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TRACER FEASIBILITY STUDY

Report No 84-20-K

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ABSTRACT

A feasibility study for a long-range tracer experiment at Nanticoke TGS is presented. The experiment involves tracking of the long-range transport of emissions from Nanticoke TGS to the Muskoka, Ontario region using the chemical tracer perfluoromethylcyclohexane. Calculation of tracer release rates, tracer release systems, air sampling and detection instruments, and sampling networks are discussed.

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To Mr. D.K.A. Gillies
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TRACER FEASIBILITY STUDY

1.0 INTRODUCTION

Chemical atmospheric tracers are usually inert, gaseous materials used to study the transport and dispersion of atmospheric pollutants. Emissions from a single specific source can be labelled with a tracer and tracked in the presence of pollutants from many sources, eg, the plume from a coal-fired generating station situated in a heavily industrialized region. The Atmospheric Research Section was requested by Central Thermal Services to carry out a feasibility study for a long-range tracer experiment at one of Ontario Hydro's thermal generating stations. An experiment designed to track the long-range transport and dispersion of emissions from Nanticoke TGS to the Muskoka, Ontario region, a distance of almost 300 km is described in the following report. Nanticoke TGS is a coal-fired generating station situated in a region containing many major sources of air pollutants. A tracer experiment would provide information with which to begin assessment of the contribution of Ontario Hydro's emissions, and associated secondary pollutants, to the sulfate aerosol and acidic precipitation deposited in the Muskoka, Ontario region.

Inert chemical atmospheric tracers were described in a recent Ontario Hydro Research Division Report/1/. Sulfur hexafluoride (SF_6) was recommended for use in short-range (< 100 km) plume tracking experiments and in longer range studies only if background concentrations are very low. Perfluoromethylcyclohexane (PMCH) and perfluorodimethylcyclohexane (PDCH) were recommended for use in long-range (>100 km) plume tracking experiments. PMCH was therefore the tracer chosen for this study.

The following report presents the results of the feasibility study. The report is divided into two parts, the first part describes the perfluorocabon tracer PMCH, methods of tracer release, sample collection and analysis. Dispersion formulae for calculation of the amount of tracer to be released are presented and the meteorological data required are also discussed. Part two presents information specific to carrying out the tracer experiment at Nanticoke TGS, eg, tracer release rates, sampler network, meteorological conditions needed, etc. The data collected from the tracer study can also be used to calculate the vertical and horizontal plume dispersion parameters, σ_y and σ_z, respectively. This is discussed in Section 6.0.

2.0 PERFLUOROCARBON TRACERS

In 1980, Heffter et al/2/ reported the development of two new perfluorocarbon tracers, perfluoromethylcyclohexane (C_7F_{14}, PMCH) and perfluorodimethylcyclohexane (C_8F_{16}, PDCH). The atmospheric background concentration of PDCH is about 0.03 ppt, approximately 1/20 of the background concentration of SF_6. The background level of PMCH is another order of magnitude lower. The amount of PDCH which must be released in an experiment, to distinguish the plume from background at the maximum sampling distance, is about 10% of that for SF_6 and for PMCH it is about 1% of the SF_6 rate. Taking the higher price of perfluorocarbons into account, the PDCH required for an experiment would cost about 20% more than SF_6, the cost of PMCH would be about 10% of the SF_6 cost/3/. Perfluoromethylcyclohexane was the chemical tracer used in the recent CAPTEX '83 field study/4,5/, and is the perfluorocarbon tracer considered in this feasibility study.

2.1 PMCH Release

Perfluoromethylcyclohexane (PMCH) is a colourless liquid at room temperature (d 1.79 g/mL, bp 76.14°C), and must be released by either atomization or vaporization followed by dilution, to prevent condensation. The vapours must be diluted until they are below the ambient dew point concentration/6/. The release system used in the CAPTEX '83 study was trailer-mounted and completely self-contained (no air compressor required). The system consisted of a metal tank containing the tracer, four pressurized N_2 cylinders, a tube furnace, a generator and fuel tank, a mass flow meter, a stripchart recorder and a large set of crane scales (0-450 kg). PMCH was shipped from England in 10-kg containers and transferred to the tank on the trailer. The cost of PMCH was about $100/kg (US, 1983). The tracer release procedure is as follows: PMCH is mixed with a stream of N_2 to evaporate it and carry the tracer through the system. This mixture of N_2 and PMCH gas flows into the tube furnace where the tracer is vaporized. The temperature of the furnace is kept above 105°C to assure complete vaporization. The mixture of N_2 and PMCH then passes through a mass flow meter where the volume is metered. From there the tracer is released to the atmosphere, at ground level, via a short (<30 cm) metal pipe. The mass flow meter provides both instantaneous and total volumes and also supplies a 0-5 volt dc output which is connected to a strip chart recorder. The recorded release rate shows the constancy of tracer release and provides a measurement of total output over the time of release. The scales provide accurate weighings of the tracer tank before and after release/5/.

2.2 PMCH Sample Collection and Detection

Perfluoromethylcyclohexane is sampled from the air by an adsorption process. A programmable adsorbent sampler was developed by Dietz at Brookhaven/6/ and is commercially manufactured for the National Oceanic and Atmospheric Administration (NOAA) by Gilian Instrument Corporation as the Brookhaven Atmospheric Tracer Sampler (BATS).

The sampler consists of an air flow module (lid) and a power control module (base). The entire unit measures 36x25x20 cm and weighs 7 kg. The lid contains 23 sampling tubes filled with 150 mg Ambersorb (trade name Rohm and Haas Company) which traps all perfluorocarbons in the air flowing through the tube. The base contains a constant volume pump which draws air through each sampling tube in a sequence controlled by an internal digital clock. Flow rates, controlled by critical orifices, can be varied from 2 to 5 mL/min. The base also contains a digital printer that records the tube number, start time and number of pump strokes (which can be converted to air volume) for each sample. Controls in the base provide for automatic start at a preselected day and time/7/. Eighty BATS samplers were employed during the CAPTEX '83 study. Six consecutive six-hour samples, total duration 36 hours, were collected for each CAPTEX tracer release/5/. When sampling is complete, the tubes are returned to the laboratory for analysis. The sample tubes are heated to 400°C to release the adsorbed materials. The recovered constituents pass through a palladium catalyst bed (3% Pd supported on a 5A molecular sieve) to remove and destroy interfering components, eg, oxygen and chlorofluorocarbons, which are present in the air at concentrations an order of magnitude higher than that of PMCH. The bed temperature is maintained above 220°C. The interfering constituents are reduced by H_2 in the 5% H_2 in N_2 carrier gas. Only PMCH and SF_6 survive. The sample then passes through a gas chromatograph column and enters a ^{63}Ni electron capture detector. This detector provides a measurement accuracy within 10% at concentrations as low as 0.002 ppt (the approximate ambient concentration of PMCH)/6/.

3.0 SAMPLING NETWORK

The number of samplers available for a field study is usually a primary constraint in network sampler design. For a given number of samplers, two conflicting considerations must be balanced:

- angular width of the sampler array relative to the tracer release point must be maximized in order to maximize the frequency of wind directions that will take the tracer from the release point to the sampler array;

- angular distance between the samplers must be minimized in order to maximize the spatial resolution of the plume measurements; adequate plume definition usually requires that samples be collected from at least five locations lying between the $\pm 2\sigma$ points of the plume concentration distribution/8/. An important consideration is that the number of sampler arcs at different downwind distances meet the objectives of the field study, ie, is plume dispersion to be characterized at only one downfield distance requiring only one sampler arc. Generally 90° is considered the minimum angular width of the sampler arc since for smaller arc widths, the normal wind direction is likely to take the tracer off the sampler grid with unacceptable frequency/8/. In designing a tracer sampler layout for obtaining hour-average tracer data, primary consideration must be given to the minimum hour-average plume width associated with the meteorological conditions of interest.

In the CAPTEX '83 study, the operational plan was to track the dispersion of a plume of PMCH tracer over a distance of approximately 1000 km. The sampling network consisted of 80 stationary ground-based samplers and seven aircraft equipped with samplers. The ground-based samplers were arranged in arcs at approximately 100 km intervals from 300 to 1100 km from the Ohio release point. The samplers in the aircraft were used to collect data on the vertical distribution of the tracer at various times after release.

4.0 CALCULATION OF AMOUNT OF TRACER TO BE RELEASED

The amount of tracer released and the rate of release are usually determined by optimization of two basic criteria:

- cost of the tracer material
- ambient concentration required at any sampling location.

The minimum acceptable release rate for an atmospheric experiment is a function of the following factors:

- sampling location (height, range, bearing)
- wind speed
- atmospheric diffusion (surface roughness, atmospheric stability, mixing depth)
- background concentration (χ_{bkg})
- instrument detection threshold (C_{min}) and dynamic range
- sampling duration
- objective of the experiment (ie, simulation of puff or continuous dispersion).

Calculation of the necessary minimum release rate requires (i) estimation of the minimum ambient concentration (χ_{min}) that must be "produced" to provide an acceptable signal-to-noise ratio in the detection instrument at the most distant sampling point; and (ii) estimation of atmospheric dispersion.

The minimum ambient concentration (χ_{min}) is defined as the product of the background concentration (χ_{bkg}) of the chemical to be released or the minimum concentration (C_{min}) required by the detection instrument, whichever is highest, and a safety factor, k, equation 1.

$$\chi_{min} = k \text{ MAX } (\chi_{bkg}, C_{min}) \qquad (1)$$

A safety factor (k ~10) must be applied due to the uncertainties in the various dispersion parameters. The determination of χ_{min} will vary according to the nature of the experiment. For studies of plume dispersion from a single isolated source it can be practically

expressed as the concentration two standard deviations from the maximum concentration (χ_{peak}) on the plume centreline.

$$\chi_{min} \tilde{=} 0.1\ \chi_{peak} \qquad (2)$$

$$\chi_{peak} \geq 100\ \text{MAX}\ [\chi_{bkg}, C_{min}] \qquad (3)$$

Atmospheric dispersion can be estimated using the Gaussian plume diffusion model equation 4/9/.

$$\chi_{(x,y,z;H)} = \frac{Q}{2\pi\sigma_y\sigma_z U} \exp\left[\frac{-y^2}{2\sigma_y^2}\right]\left\{\exp\left[\frac{-(z-H)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z+H)^2}{2\sigma_z^2}\right]\right\} \qquad (4)$$

where: $\chi_{(x,y,z;H)}$ = concentration of gas (or aerosol) at a point x,y,z

H = effective emission height (see Appendix A)

σ_y = standard deviation of plume concentration distribution in the horizontal

σ_z = standard deviation of plume concentration distribution in the vertical

U = mean wind speed affecting the plume

Q = emission rate

The last term, $\exp\left[\frac{-(z+H)^2}{2\sigma_z^2}\right]$, accounts for reflection of the plume at the ground by assuming an image source at distance H, beneath the ground surface. χ is a mean over the same time interval as that for which the σ's and U are representative. σ_y and σ_z vary with turbulent structure of the atmosphere, the height above the surface, surface roughness, sampling time over which the concentration is to be estimated, wind speed and the distance from the source. For calculation of the concentrations at ground level, z=0, equation (4) simplifies to:

$$\chi_{(x,y,0;H)} = \frac{Q}{\pi\sigma_y\sigma_z U} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \exp\left[-\frac{H^2}{2\sigma_z^2}\right] \qquad (5)$$

When the ground-level concentration is to be calculated along the plume centreline (y=0, z=0) further simplification is possible:

$$\chi_{(x,0,0;H)} = \frac{Q}{\pi\sigma_y\sigma_z U} \exp\left[-\frac{H^2}{2\sigma_z^2}\right] \qquad (6)$$

The vertical and horizontal dispersion, σ_y and σ_z, respectively, can be estimated as a function of downwind distance from the source, x. A stable layer existing above an unstable layer will restrict vertical diffusion. The dispersion computation can be modified by considering the height of the base of the stable layer, L. At a distance x_L, defined as the point where σ_z has a value of 0.47 L, the plume is assumed to have a Gaussian distribution in the vertical. After the plume has travelled twice this far, $2x_L$, it is assumed to have become uniformly distributed between the earth's surface and the base of the stable layer, L, ie, concentration does not vary with height. For distances greater than 2 x_L, the concentration for any height between the ground and L can be calculated from:

$$\chi_{(x,y,z;H)} = \frac{Q}{\sqrt{2\pi}\sigma_y LU} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \qquad (7)$$

for any z from 0 to L;

for $x > 2x_L$; x_L is where $\sigma_z = 0.47$ L.

With respect to σ_y, at large distances the Fickian and Taylor theories of diffusion predict that σ_y is proportional to $x^{1/2}$/10/. In 1965 Heffter/11/ reported the results of his investigation of the relationship

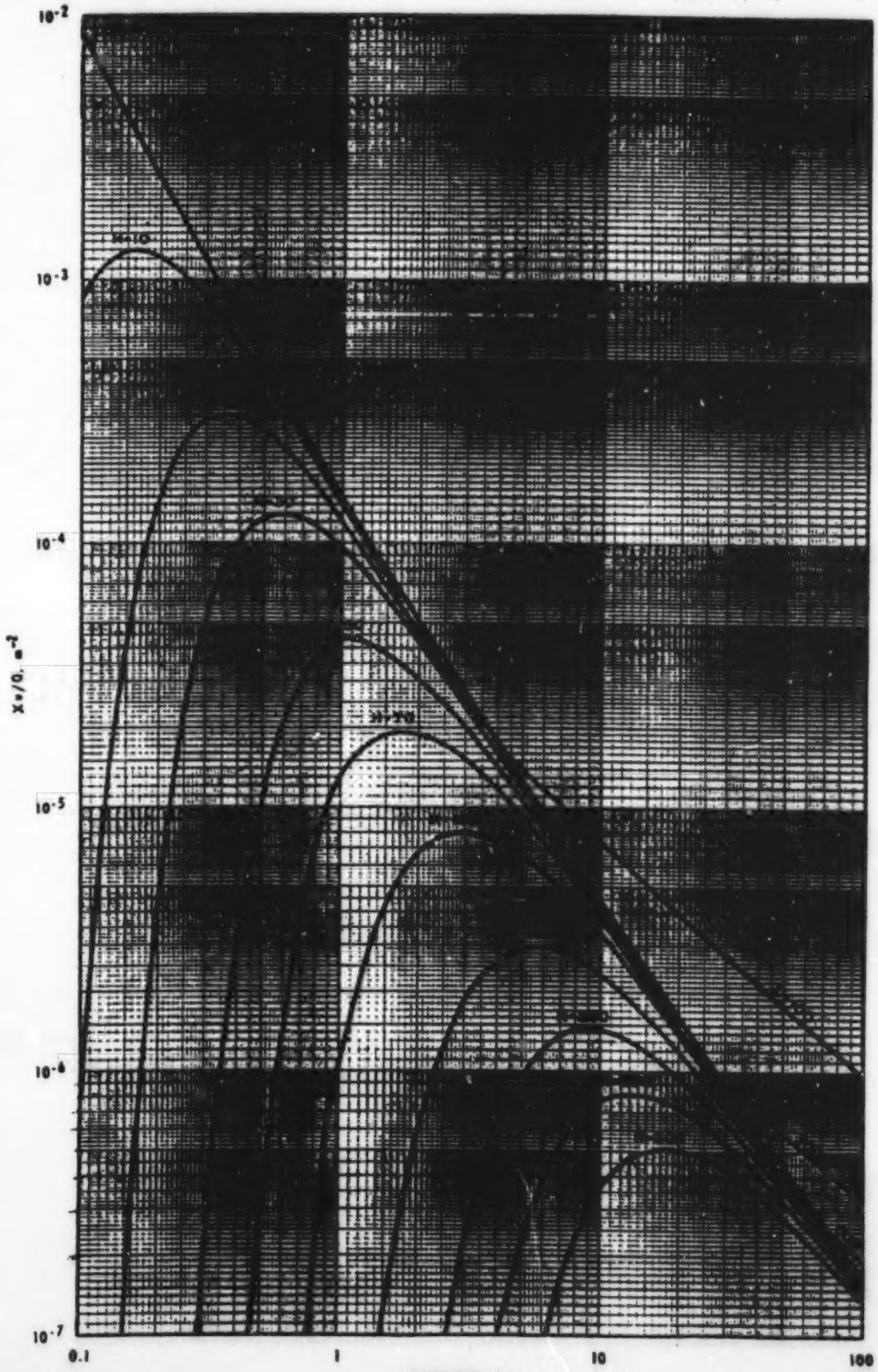
$$K_h = \sigma_y^2/2t \qquad (8)$$

where K_h is the horizontal coefficient of eddy diffusion for travel periods (t). The study involved collection, evaluation and combination of as many of the published diffusion measurements (σ_y) as applicable. Only measurements of σ_y for travel periods of longer than 1 h were considered. The scarcity of data during the 4 to 12 h period combined with the scatter of data points for shorter travel periods made determination of a meaningful general relationship regarding the variation of σ_y or K_h with time during the period of 12 to 24 h difficult. However, there appeared to be little change in K_h with time from about 24 to 96 h. Heffter suggests that an average value of $K_h \sim 4 \times 10^8$ cm^2 s^{-1} will apply to dilution estimates with associated travel periods of 1-4 days. This value for K_h can, however, vary considerably; reliable values lower by about a factor of 10 have been observed.

To simplify calculation of ground-level concentrations, graphs (Turner's Tables) illustrating the variation of normalized ground-level plume centreline concentrations as a function of range (x), effective source height (H), mixing layer depth (L) and stability are available/9/, see Figure 1. The graphs are based on calculations using equations 5 and 6. The values of parameters σ_y and σ_z used to generate Turner's Tables are derived from a few diffusion experiments performed during the 1950's and 1960's. The experiments were carried out over relatively uniform terrain, the height was assumed to be the

FIGURE 1

χU/Q WITH DISTANCE FOR VARIOUS HEIGHTS OF EMISSION (H) AND LIMITS TO VERTICAL DISPERSION (L), D STABILITY/19/



lowest several hundred meters of the atmosphere, sampling times of about 10 minutes were used and concentrations were measured at downwind distances of less than 1 km/10/. Beyond 1 km the concentrations were estimated. As a result, values calculated for σ_y and σ_z, and hence the results presented in Turner's Tables, can only reliably be applied to very short plume travel distances (<100 km) and under a limited set of meteorological/topographical conditions.

To calculate ground-level concentrations after longer plume travel distances (>100 km) equation 7 must be used.

To estimate the amount of tracer to release and the rate of release, for a long-range transport study, equation 3 would be substituted into equation 7 to give equation 9. This would be solved for the appropriate values.

$$\chi_{(x,0,0;H)} = \frac{Q}{2\sqrt{K_h t \pi}\ L\ U} \qquad (9)$$

A sample calculation of the release rate required for a long-range PMCH tracer study is given in Section 5.2.

5.0 TRACER STUDY AT NANTICOKE TGS

Nanticoke TGS, a coal-fired station, is located in southwestern Ontario, on the north shore of Lake Erie near Simcoe, Ontario. The topography is predominantly flat (gradient 2.5 m/km extending at least 20 km inland) and dominated by agricultural activity. A major oil refinery is located about 2 km north of the power plant and a steel mill lies about 5 km to the west. The purpose of a tracer study at this station is to track the long-range transport and dispersion of emissions from Nanticoke TGS to the Muskoka, Ontario region, a distance of almost 300 km. Monitoring of the dispersion of tracer as a function of distance and time will provide information with which to begin assessment of the contribution of emissions from Nanticoke TGS to the SO_2, sulfate aerosol and acidic precipitation observed in this region.

Nanticoke TGS has a total maximum capacity of 4040 MW. The station has two stacks, each having a height 198.1 m above grade. There are four flues per stack and the flue outlet diameter is 5.49 m. The flue gas exit velocity at full load is 27.4 m s^{-1} and the flue gas exit temperature at full load is 138°C. Winds from the south-southwest transport emissions from Nanticoke TGS north-northeast in the direction of the Muskoka, Ontario region.

5.1 Sampling Network

Design of a tracer sampling network was discussed in Section 3.0. The geography of the Great Lakes restricts the angle of an arc of samplers, 300 km from Nanticoke TGS, to 62° (length of arc is 324 km). The major limitation to the density of the sampling points within this sector is the number of perfluoromethylcyclohexane samplers (BATS)

available. In a tracer study using the perfluorocarbons PDCH and PMCH, carried out by NOAA/7/, 30 sampling sites were selected at 4-5 km (~2°) intervals along a 75° arc, 100 km from the release site. Only seventeen samplers were actually available, therefore the sites to be instrumented were selected immediately prior to the start of the tracer release. The small size of the perfluorocarbon samplers permits this type of portability. The Atmospheric Research Section does not own any perfluorocarbon samplers. The size of the sampling network will therefore depend upon the number of samplers which can be borrowed (3 from OME, 4-5 from AES) and/or rented from the National Oceanic and Atmospheric Administration (NOAA). Therefore, as in the NOAA study, the samplers will have to be positioned, at preselected sampling sites, immediately prior to the release of the tracer. A network consisting of two arcs of samplers located 200 and 300 km north-northeast of Nanticoke TGS is proposed. Sampling sites would be chosen at 2° intervals along the arcs. Estimates of sampler separation on the basis of having at least five samplers lying between the $\pm 2\sigma$ points of the plume concentration distribution/8/, where $\sigma_y = \sqrt{2K_h t}$/11/, suggest that 4-5° intervals between the samplers are required. If 2° intervals are used, the 300 km arc would consist of 31 potential sampling sites located at approximately 10-km intervals. The 200-km arc would subtend a 50° angle, see Figure 2. Twenty-five potential sampling points would be spaced at 7-km intervals along this arc. If the availability of instruments restricts sampling to a single arc, the arc should be located approximately 300 km NNE of Nanticoke TGS. In addition to the PMCH samplers, SO_x and NO_x monitoring equipment would be positioned at various points along the sampling arc(s).

5.2 PMCH Release

Dispersion formulae with which to calculate the amount of tracer to release were presented in Section 4.0. For dispersion over long distances, equation 7 is used.

$$X_{(x,y,z;H)} = \frac{Q}{\sqrt{2\pi}\ \sigma_y\ LU} \exp\left[\frac{-y^2}{2\sigma_y^2}\right] \qquad (7)$$

for any z from 0 to L

for $x > 2x_L$; x_L is where $\sigma_z = 0.47\ L$.

After long travel times σ_y is equal to $\sqrt{2K_h t}$ where K_h is the horizontal coefficient of eddy diffusion and t is the travel time/11/. To calculate the maximum ground-level concentration along the plume centreline, y=0, z=0, equation 7 simplifies to:

$$X(x,0,0;H) = \frac{Q}{2\sqrt{K_h t \pi}\ LU} \qquad (9)$$

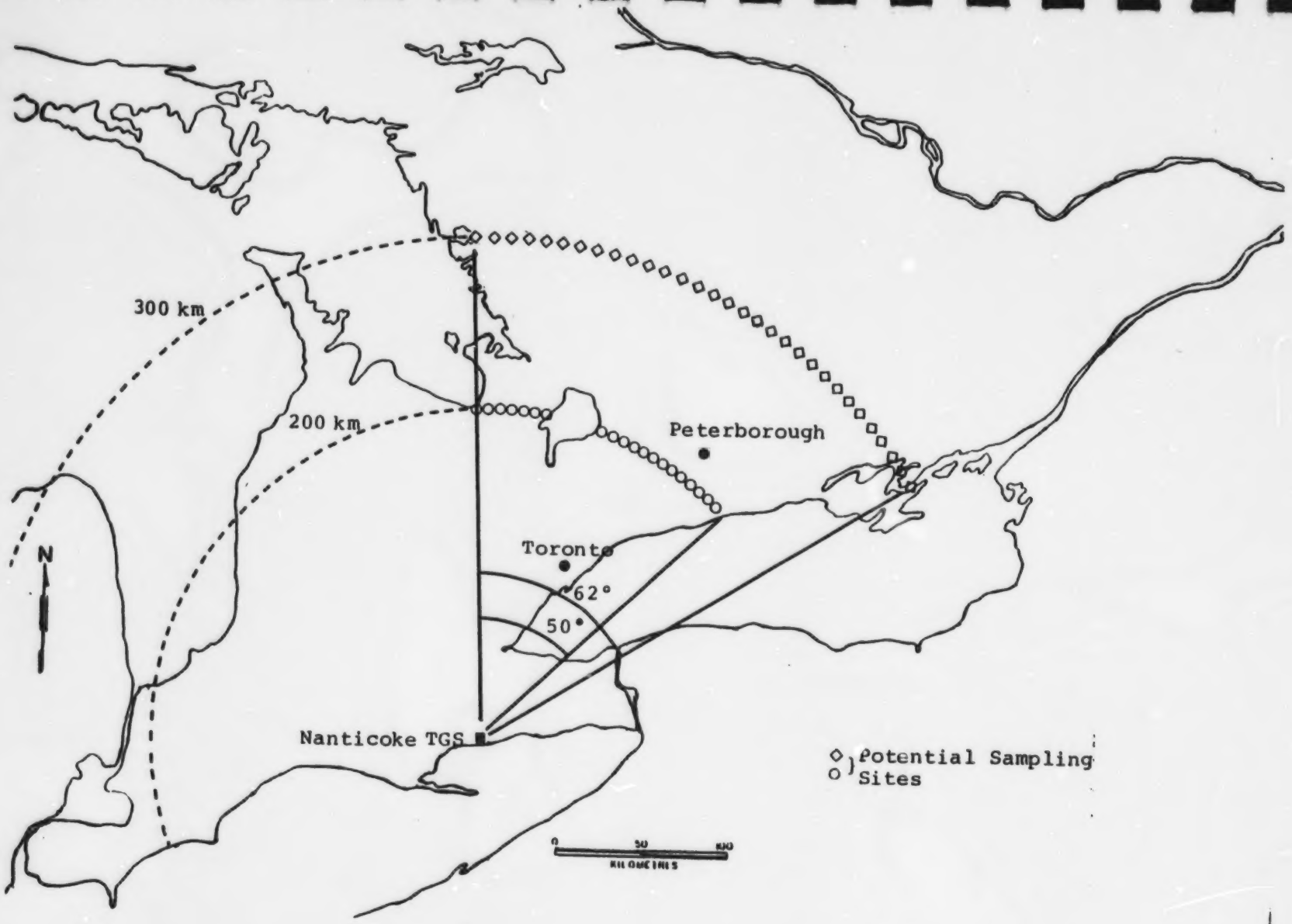


FIGURE 2

PROPOSED SAMPLING SITES FOR A PMCH
TRACER STUDY BASED AT NANTICOKE TGS

A sample calculation of PMCH release rate from Nanticoke TGS is shown below. The following conditions are assumed:

- wind speed (U) = 5 m s^{-1};
- height of boundary layer (L) = 500 m;
- maximum downwind sampling location (x) = 3×10^5 m;
- plume travel time = 6×10^4 s;
- instrument detection limit (C_{min}) = 0.002 ppt = 2.86×10^{-8} mg m^{-3};
- PMCH background concentration (χ_{bkg}) = 0.004 ppt = 5.73×10^{-8} mg m^{-3};
- $K_h = 4 \times 10^8$ cm^2 s^{-1} = 4×10^4 m^2 s^{-1}.

Recall from Section 4.0, the minimum concentration to be detectd at the maximum downwind sampling location is given by equation 1.

$$\chi_{min} = 100 \text{ MAX } [\chi_{bkg}, C_{min}] \qquad (1)$$

In CAPTEX '83 a safety margin of 3 orders of magnitude was used.

Therefore,

$$\chi_{min} = 1000 \text{ MAX } [\chi_{bkg}, C_{min}] \qquad (10)$$

Substituting equation 10 into equation 9,

$$1000 \text{ MAX } [C_{min}, \chi_{bkg}] = \frac{Q}{2\sqrt{K_h t \pi}\ LU}$$

$$Q = 1000 \text{ MAX } [C_{min}, \chi_{bkg}] \cdot 2\sqrt{K_h t \pi} \cdot LU \qquad (11)$$

Therefore, the PMCH release rate estimate is

$$Q = 1000 \times 5.73 \times 10^{-8} \text{ (mg } m^{-3}) \times 2\sqrt{4 \times 10^4 \text{ } (m^2\ s^{-1}) \times 6 \times 10^4 (s) \times \pi \times 500 \text{ (m)} \times 5 \text{ (m } s^{-1})}$$

$$= 2.49 \times 10^4 \text{ mg } s^{-1}$$

$$= 90 \text{ kg } h^{-1}$$

This release rate can be compared with PMCH release rates used in previous perfluorocarbon tracer experiments. In the NOAA study/7/ 192 kg of PMCH were released over a period of 3 h (64 kg h^{-1}) and tracked for a distance of 600 km. During the CAPTEX '83 study, about 200 kg of PMCH were released over a 3-h period (67 kg h^{-1}) and tracked over distances of at least 600 km/5/. The rates of PMCH release used in these studies were calculated using a procedure similar to that outlined above, ie, calculation of χ_{bkg}, C_{min} and substitution into the Gaussian diffusion model/12/. The actual release rates were, however, generally higher than those calculated, the amount by which the release rates were increased was based upon information gathered during a number of preliminary field studies. C.R. Dickson/12/, on the basis of his experience with tracer field studies, suggested that a release rate of about 50 kg h^{-1} for the Nanticoke TGS experiment would probably suffice.

Release of the perfluorocarbon tracer requires a system similar to that used in the CAPTEX '83 study and described in Section 2.2. The perfluorocarbon would be injected via a stainless steel probe into the stack, this is in contrast to the ground-level releases during the CAPTEX '83 study. The tracer should be injected into the duct after the ID fan, at one of the ports used for stack gas sampling.

As discussed earlier, air samples would be collected using BATS samplers. The BATS samplers contain 23 sampling tubes and can be programmed to sample air at a rate from 1 minute to 1 week per tube. In the NOAA study/7/ the samplers were set to collect 22 3-h samples.

5.3 Meteorological Conditions Required for the Nanticoke TGS Tracer Study

Tracking of a chemical tracer released from Nanticoke TGS to the Muskoka, Ontario region, a distance of approximately 300 km requires careful examination of synoptic weather conditions to ensure that the tracer is transported in the direction of interest. The source-receptor relationship between Nanticoke TGS and the Muskoka-Huntsville, Ontario area is very complex. It can, however, be simplified to the extent that the transport of emissions is primarily a function of synoptic weather conditions. The Muskoka-Huntsville area is located north of Nanticoke TGS. Winds from the south will, therefore, carry emissions from Nanticoke TGS to this region. Southerly winds in the Nanticoke area could occur under the following conditions:

(1) when a center of high pressure is located to the south or east of the lower Great Lakes;

(2) when a center of low pressure is located over or to the north of the upper Great Lakes;

(3) when a warm front moves into the Nanticoke area from the south;

(4) any combination of (1),(2) and (3).

Table I presents the frequency of occurrence of southerly wind events in 1981 and the synoptic weather situation for each event. Most southerly wind events occur when a center of high pressure is located south or east of Nanticoke and a front passes over the area.

TABLE I

FREQUENCY OF OCCURRENCE OF SOUTHERLY WIND EVENTS IN 1981 AND THEIR SYNOPTIC WEATHER SITUATIONS

Month	No of Events	Synoptic Weather Situation			
		High	Low	Front	Combination
Jan	8	3	1	3	1
Feb	10	3	0	6	1
Mar	7	4	2	1	0
Apr	13	5	6	1	1
May	6	1	0	4	1
Jun	7	3	1	3	0
Jul	4	2	0	2	0
Aug	4	2	0	1	1
Sept	6	1	0	4	1
Oct	7	4	0	3	0
Nov	8	5	0	3	0
Dec	13	4	0	7	2
Total	93	37	10	38	8
Percentage	100	40	11	41	8

A high pressure system is generally associated with fair weather. Winds are light and there is no precipitation. Dry deposition is the primary mechanism by which acidic deposition occurs as emissions move from source to receptor. A system of low pressure is associated with unsettled weather. Winds are relatively strong, skies are cloudy and precipitation occurs in the form of rain or snow. Transport of emissions from source to receptor is more complicated and deposition can involve dry and wet processes. In addition, the transport and

transformation of pollutants which occurs within clouds must be considered. Transport of emissions from Nanticoke TGS to the Muskoka area is faster in a low pressure system relative to a high pressure system. Duration of transport from Nanticoke TGS to Muskoka depends upon the strength of the pressure system and whether or not the system is stationary. For example, in 1981 weather maps revealed that a high pressure system took from 1 to 2 days to pass through the area of interest, an isolated release of tracer may take less time. Had a tracer study been conducted in 1981, it should have been in late fall or winter, when the probability of southerly winds was the highest, see Table I. A winter field study could, however, pose many problems with respect to positioning and manning of the samplers in snow and operation of the samplers in cold weather.

5.4 Interpretation of Data

Data collected during the Nanticoke TGS study will include:

(1) concentrations of perfluoromethylcyclohexane as a function of time and distance from Nanticoke TGS;

(2) air and precipitation pollutant concentrations (eg, $[SO_2]$, $[SO_4^{2-}]$, $[NO_x]$, $[HNO_3]$ in air; $[SO_4^{2-}]$, $[NO_3^-]$, $[H^+]$ in precipitation) as a function of time and distance from Nanticoke TGS;

(3) initial concentrations of PMCH, SO_2, NO_x, etc emitted from Nanticoke TGS;

(4) related meteorological data.

Analysis of these data will yield information about whether or not, under the meteorological conditions which existed during the study period, emissions from Nanticoke TGS were transported to the Muskoka area. Estimates of Ontario Hydro's contribution to pollution in this region based on the collected data can only be very crude because the rates of deposition and chemical transformation of PMCH are very much slower than those of SO_2, SO_4^{2-}, NO_x etc.

6.0 ESTIMATION OF σ_y AND σ_z

In addition to estimation of Ontario Hydro's contribution to ground-level pollution concentrations in the Muskoka, Ontario region, the data collected during the tracer studies can be used to calculate the lateral and vertical plume dispersion parameters, σ_y and σ_z, respectively. Two methods have been used to estimate these functions: (1) direct calculation of the second moment of the measurements, and (2) calculation of the value of each function that provides the best fit to the assumed concentration distribution. These two methods are summarized below. For a more detailed discussion the reader should refer to reference 6.

The second moment or standard deviation of the horizontal concentration distribution is calculated using equation 12,

$$\sigma = \left(\frac{\Sigma \chi y^2}{\Sigma \chi} \right)^{1/2} \qquad (12)$$

where y is the distance from the plume centreline and χ is the corresponding value of the observed concentration. When the sampling line is not perpendicular to the plume centreline a simple adjustment involving a mathematical rotation of the sampling line is required.

The second method for calculation of σ_y involves a number of steps, the sequence of steps is outlined in the following:

(1) All hourly concentration profiles are represented as arrays of: tracer concentration, range (from release point); and bearing.

(2) The profiles are analyzed to obtain a first estimate of the plume centreline position and standard deviation.

(3) The initial arrays (step 1) are adjusted by mathematically rotating the orientation of the sampling lines so they are perpendicular to the plume centreline (step 2); steps (2) and (3) are repeated until there is no significant change in the plume centreline position.

(4) Using the final estimate of plume centreline position and the corresponding adjusted data arrays, the (adjusted) hourly profiles for multiple tracer distributions are analyzed.

The standard deviation is calculated using a linearization-of-function technique based on a Taylor expansion of a nonlinear function, $f(m)$. A gradient search method is used to minimize Chi-square (χ^2_{fit}, the goodness of fit).

$$\chi^2_{fit} \equiv \left\{ \frac{1}{\sigma_i^2} \left[f_i - f(m_i) \right]^2 \right\} \qquad (13)$$

where f_i is the observed value of the variable (eg, tracer concentration) and $f(m_i)$ is the value of the variable calculated for m_i from the nonlinear function. The curve fitting routine requires two subjective choices: the function to be fit and an "initial guess" of the fit. The data are then fit to a multiple Gaussian distribution with zero background, equation 14.

$$\chi = \sum_{i=1}^{q} \chi_{peak_i} \exp\left[-\frac{(y-\bar{y})^2}{2\sigma_i^2}\right], q = 1,2 \text{ or } 3 \qquad (14)$$

where χ_{peak} is the centreline or peak concentration, y is the crosswind distance from the centreline position ($\bar{y}$); σ is the standard deviation of the Guassian distribution; and q is the number of peaks (the number is determined subjectively by first reviewing the composite hourly profiles).

σ_z, the vertical diffusion parameter is more difficult to determine because of plume impingement at the ground surface and elevated inversions. Dabberdt et al/6/ reported a method that uses the linearization-of-function routine described earlier and the crosswind integrated form of the Gaussian plume equation. This approach is independent of σ_y calculations as χ_{cwi} (crosswind-integrated concentration) is calculated directly from the observations. The point source Gaussian plume equation used is

$$\chi = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left[-\tfrac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\tfrac{1}{2}\left(\frac{z-h}{\sigma_z}\right)^2\right] + \exp\left[-\tfrac{1}{2}\left(\frac{z+h}{\sigma_z}\right)^2\right] + \exp\left[-\tfrac{1}{2}\left(\frac{z-2H-h}{\sigma_z}\right)^2\right]\right\} . \qquad (15)$$

Equation 15 is integrated along y to give the crosswind integrated form of the plume equation:

$$\chi_{cwi} \equiv \int_{-\infty}^{+\infty} \chi dy = \frac{Q}{\sqrt{2\pi}\sigma_z\bar{u}}\left\{\exp\left[-\tfrac{1}{2}\left(\frac{z-h}{\sigma_z}\right)^2\right] + \exp\left[-\tfrac{1}{2}\left(\frac{z+h}{\sigma_z}\right)^2\right] + \exp\left[-\tfrac{1}{2}\left(\frac{z-2H-h}{\sigma_z}\right)^2\right]\right\} \qquad (16)$$

where χ_{cwi} has units of g m^{-2}. Equation 16 has been used to solve simultaneously for the terms σ_z and $\frac{Q}{\sqrt{2\pi}\ \sigma_z \bar{U}}$.

7.0 COSTS

Two important factors control the cost of the long-range PMCH tracer study, (i) the number of tracer releases required and (ii) the number of sampling instruments which can be borrowed or rented. During the CAPTEX '83 study, 3-3h tracer releases were planned from each of the two sites. If 3-3h PMCH releases are planned from Nanticoke TGS, approximately 600-800 kg of PMCH would be required. In 1983 the cost of PMCH was $100 (US)/kg. The cost of the tracer would therefore range between $60 and $80 K. With respect to samplers, a minimum of 15 are needed, see Section 5.1. A total of 8 may be available from AES and OME. Arrangements would have to be made to borrow or rent the remainder, ie, from NOAA. The approximate purchase cost of a sampler is $10 K.

In addition to the costs described above, other costs to consider include sample analysis, construction of the tracer release system and labour.

8.0 CONCLUSIONS

A feasibility study for a tracer experiment at one of Ontario Hydro's power plants has been presented. The experiment involved tracking of the long-range transport of emissions from Nanticoke TGS to the Muskoka, Ontario region using perfluoromethylcyclohexane. The feasibility study examined tracer release systems, air sampling and detection instruments and sampling networks. The tracer would be released out of the top of the power plant stack. The required rate of tracer release was estimated using the Gaussian plume dispersion model. Calculations suggest a release rate from Nanticoke TGS of about 90 kg h^{-1}.

9.0 RECOMMENDATIONS

The release, sampling and analytical techniques required for a perfluorocarbon tracer study are relatively new and the chemicals and samplers needed are not readily available. It is recommended that planning of a perfluorocarbon tracer study at Nanticoke TGS be delayed until the results (and recommendations) of the latest perfluorocarbon tracer study (CAPTEX '83) become available.

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REFERENCES

1. KALVINS, A., 1983. "Chemical Atmospheric Tracers," Ontario Hydro Research Division Report No 83-212-K.

2. HEFFTER, J.L., G.J. Ferber and P.W. Krey, 1980. "Atmospheric Tracer Experiments for Regional Dispersion Studies," Proc Semin Radioact Releases Their Dispersion Atmos Hypothetical React Accid 2, 953.

3. LOVELOCK, J.E., and G.J. Ferber, 1982. Atmos Environ 16, 1467 and references therein.

4. KALVINS, A., 1983. "Cross-Appalachian Tracer Experiments, CAPTEX '83", Ontario Hydro Research Division Report No C83-67-K.

5. EDWARDS, G.C. and A. Kalvins, 1983. "CAPTEX '83 Sudbury Release Site Visit," Ontario Hydro Research Division Report No C83-138-K.

6. DABBERDT, W.F., and R.N. Dietz, "Gaseous Tracer Technology and Applications," American Meteorological Society Short Course on Instruments and Techniques for Probing the Atmospheric Boundary Layer, Lecture Notes, August 8-12, 1983, Boulder, Colorado and references therein.

7. FERBER, G.J., K. Telegadas, J.L. Heffter, C.R. Dickson, R.N. Dietz and P.W. Krey, January, 1981. "Demonstration of a Long-Range Tracer System Using Perfluorocarbons," Final Report, EPA-600/7-81-006.

8. JOHNSON, W.B., 1983. J of Climatology and Applied Meteorology 22, 931.

9. TURNER, D.B., 1969. Workbook of Atmospheric Dispersion Estimates, US Department of Health, Education and Welfare, Public Health Service Publication No 999-AP-26.

10. HANNA, S.R., G.A. Briggs and R.P. Hosker, 1982. "Handbook on Atmospheric Diffusion," US Department of Energy DOE/TIC-11223.

11. HEFFTER, J.L., 1965. J of Applied Meteorology 4, 153.

12. DICKSON, C.R., Director, Air Resources Laboratories Field Research Division, NOAA, personal communication.

APPENDIX A

ESTIMATION OF EFFECTIVE HEIGHT OF EMISSION

When the tracer is to be released from an elevated source, $h \neq 0$, calculation of dispersion of the tracer/flue gases, requires estimation of the effective stack height or effective height of emission, H. It is defined as the sum of the physical height of the stack h_s, plus the plume rise, Δh, equation 17.

$$H = h_s + \Delta h \tag{17}$$

Plume rise can typically increase the effective stack height by a factor 2 to 10 times the actual release height. Maximum ground-level concentration is roughly proportional to the inverse square of the effective stack height, as a result, plume rise can reduce ground-level concentrations by a factor of as much as 100. The formula for the final rise of a buoyant plume, Δh, is well known:

$$\Delta h = 2.6 \left(\frac{F_o}{US} \right)^{1/3} \tag{18}$$

where F_o = the initial buoyancy flux ($m^4\ s^{-3}$)

U = mean ambient wind speed, ($m\ s^{-1}$)

S = atmospheric stability (ie, Brunt Vaisalla frequency)

The coefficient 2.6 was chosen on the basis of comparisons with many observations/10/. The initial buoyancy flux is defined by the following equation:

$$F_o = \frac{g}{T_{po}} \left(T_{po} - T_{eo} \right) V_o \quad R^2 \tag{19}$$

where:

- the subscripts p,e, and o indicate plume, environmental and initial values, respectively
- g = acceleration of gravity, 9.8 $m\ s^{-2}$
- V = plume vertical speed (stack exit velocity), $m\ s^{-1}$
- R = plume radius (inside diameter of stack exit), m
- T = temperature, (°K)

Environmental stability (S) is a function of the vertical temperature structure of the atmosphere and it is calculated using equation 20.

$$S = \frac{g}{T_e}\left(\frac{\partial T_e}{\partial z} + 0.01°C\right) \text{ or } \frac{g}{T_e}\left(\frac{\partial \Theta_e}{\partial z}\right) \qquad (20)$$

where $\frac{\partial \Theta_e}{\partial z}$ is the potential temperature gradient.